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Profiling and Optimization

SPEED Lecture Series

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February 1, 2022

I have a performance profile of my code. Now what?

- Look for the part that uses most computing time or memory transfer
- Observe the nature of tasks
  - DO loops/for loops?
  - How is the memory access pattern like?
  - I/O?
- Optimization techniques:
  - Make good use of compilers
  - Optimize memory access
  - Vectorization
  - Parallelization
  - I/O optimization

Important elements to look for

For serial codes:

- Hotspots
  Location (routines or lines) where most time is spent
- Loop structures
  Identify candidates for parallelization (threading and vectorization)
- Are there bottlenecks in the logical flow?
  e.g. C++ locks, mutex and futures

For parallel codes:

- MPI message passing
  Size of messages, where most communication is performed
- Load imbalance
- Overlapping of computation and communication

Do less work!

- Simplify expressions

$$x = Ace^{cy}$$

$$A = -\frac{1}{c}e^{cb}$$

$$x = -e^{c(b+y)}$$

```
b = 2.0
c = 3.0
A = -1.0/c * exp(c*b)
x = A*c*exp(c*y)
```

5 multiplications, 1 division, 2 exponentials

```
x = -exp(c*(b+y))
```

1 multiplications, 1 addition, 1 exponential

Do less work!

- Common subexpression elimination

```
x = cos(v)*(1+sin(u/2)) + sin(w)*(1-sin(u/2))
```

```
t = sin(u/2)
x = cos(v)*(1+t) + sin(w)*(1-t)
```

- Avoid expensive operations

```
y = x**2
```

```
y = x*x
```

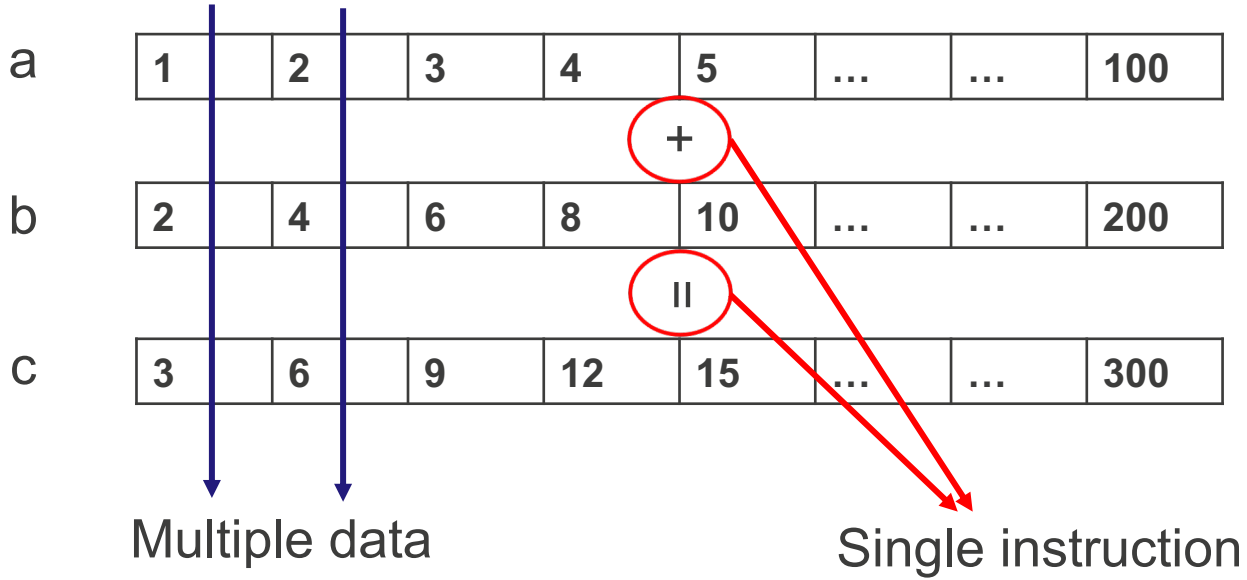
```
y = x/10
```

```
y = 0.1*x
```

Single Instruction Multiple Data (SIMD)

```
for (i=0; i<100; ++i)
   c[i] = a[i] + b[i];
```

```
DO i = 1, 100
   c[i] = a[i] + b[i]
END DO
```



Aside: Row-major order vs column-major order

Different ways to store multidimensional arrays in linear storage

- Row-major order: (C/C++, Python, Numpy)

a_{11}	a_{12}	a_{13}
a_{21}	a_{22}	a_{23}
a_{31}	a_{32}	a_{33}

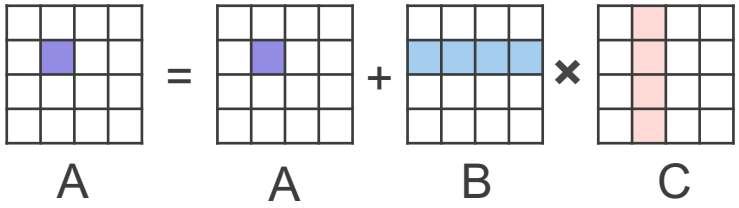
a_{11}	a_{12}	a_{13}	a_{21}	a_{22}	a_{23}	a_{31}	a_{32}	a_{33}

- Column-major order: (Fortran, MATLAB, R, Julia)

a_{11}	a_{12}	a_{13}
a_{21}	a_{22}	a_{23}
a_{31}	a_{32}	a_{33}

a_{11}	a_{21}	a_{31}	a_{12}	a_{22}	a_{32}	a_{13}	a_{23}	a_{33}

Example: Matrix-matrix multiplication



Question 1:
Are these two programs the same?

Question 2:
Which one is better? Why?

Question 3:
How can we optimize them?

Fortran 90:

```
! Matrices A, B, and C initialized

DO k = 1, N
   DO j = 1, N
      DO i = 1, N
         A(i,j) = A(i,j) + B(i,k) * C(k,j)
      END DO
   END DO
END DO
```

C++:

```
// Matrices A, B, and C initialized

for (int k=0; k<N; ++k) {
   for (int j=0; j<N; ++j) {
      for (int i=0; i<N; ++i) {
         A[i][j] += B[i][k] * C[k][j];
      }
   }
}
```

Loop reordering

Useful when you want to:

- get contiguous memory access
- vectorize on one of the indices

How will you improve the previous C++ matrix multiplication code?

```
// Matrices A, B, and C initialized

for (int k=0; k<N; ++k) {
   for (int j=0; j<N; ++j) {
      for (int i=0; i<N; ++i) {
         A[i][j] += B[i][k] * C[k][j];
      }
   }
}
```

```
// Matrices A, B, and C initialized

for (int k=0; k<N; ++k) {
   for (int i=0; i<N; ++i) {
      for (int j=0; j<N; ++j) {
         A[i][j] += B[i][k] * C[k][j];
      }
   }
}
```

Loop unrolling

Note:

Computational intensity = $\frac{\text{floating point operations}}{\text{memory operations}}$

Useful when you want to:

- increase computational intensity within a loop
- give compiler more operations to shuffle around to get more overlaps

How will you improve the previous Fortran matrix multiplication code?

```
! Matrices A, B, and C initialized
DO k=1,N
   DO j=1,N
      DO i=1,N
         A(i,j)=A(i,j) + B(i,k)*C(k,j)
      END DO
   END DO
END DO
```

```
! Matrices A, B, and C initialized
DO k=1,N-3,4
   DO j=1,N
      DO i=1, N
         A(i,j)=A(i,j) + B(i,k)*C(k,j)
                       + B(i,k+1)*C(k+1,j)
                       + B(i,k+2)*C(k+2,j)
                       + B(i,k+3)*C(k+3,j)
      END DO
   END DO
END DO
DO kk=k,N
   DO j=1,N
      DO i=1,N
         A(i,j)=A(i,j) + B(i,kk)*C(kk,j)
      END DO
   END DO
END DO
```

Avoid conditionals/branches within loops

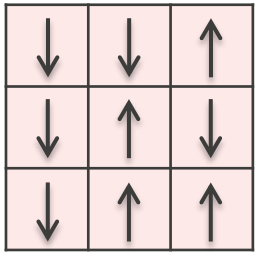
- Helps compiler vectorize the code
- For loop-independent if's:
  - remove (replace with intrinsics like `MAX`, `MIN`, `ABS`, or mathematical expressions)
  - pull them out from the loop

```
DO k=1,N
   DO j=1,N
      DO i=1,N
         IF (case==1) THEN
            A(i,j)=A(i,j) + B(i,k)*C(k,j)
         ELSE
            A(i,j)=A(i,j) + B(i,k)*D(k,j)
         END IF
      END DO
   END DO
END DO
```

```
IF (case==1) THEN
   DO k=1,N
      DO j=1,N
         DO i=1,N
            A(i,j)=A(i,j) + B(i,k)*C(k,j)
         END DO
      END DO
   END DO
ELSE
   DO k=1,N
      DO j=1,N
         DO i=1,N
            A(i,j)=A(i,j) + B(i,k)*D(k,j)
         END DO
      END DO
   END DO
END IF
```

Avoid conditionals/branches within loops

- For loop-dependent if's:
  - remove (replace with intrinsics like `MAX`, `MIN`, `ABS`, or mathematical expressions)
- Example: 2D Ising model with periodic boundary conditions



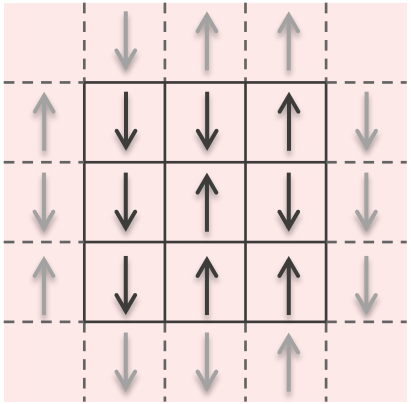
$$E = -J \sum_{<ij>} \sigma_i \sigma_j$$

```
int spin[Size][Size];
……
for (x=0; x<Size; ++x) {       // Energy calculation
   if (x!=0) xLeft = x-1;
   else xLeft = Size-1;
   for (y=0; y<Size; ++y) {
      if (y!=0) yBelow = y-1;
      else yBelow = Size-1;
      E += spin[x][y]*(spin[xLeft][y]+spin[x][yBelow]);
      M += spin[x][y];
   }
}
E *= -J;
```

How will you vectorize the energy calculation?

Avoid conditionals/branches within loops

- For loop-dependent if's:
  - remove (replace with intrinsics like `MAX`, `MIN`, `ABS`, or mathematical expressions)
- Example: 2D Ising model with periodic boundary conditions



$$E = -J \sum_{<ij>} \sigma_i \sigma_j$$

```
int spin[Size+2][Size+2];          // Create buffer halo space
for (x=0; x<Size; ++x) {           // Copy the spins to the halos
   spin[x][0] = spin[x][Size];
   spin[x][Size+1] = spin[x][1];
}
for (y=0; y<Size; ++y) {
   spin[0][y] = spin[Size][y];
   spin[Size+1][y] = spin[1][y];
}
for (x=1; x<Size+1; ++x) {         // Energy calculation
   if (x!=0) xLeft = x-1;
   else xLeft = Size-1;
   for (y=1; y<Size+1; ++y) {
      if (y!=0) yBelow = y-1;
      else yBelow = Size-1;
      E += spin[x][y]*(spin[x-1][y]+spin[x][y-1]);
      M += spin[x][y];
   }
}
E *= -J;
```

Loop splitting

- Useful when you want to:
  - remove non-vectorizable components from large computational loops
  - split non-tightly nested loops
- Caveat: does not always work because it increases memory movements

```
cmax = 0.0; imax = -1;
for (i=0; i<1000000; ++i){
   ctmp = a[i] + b[i];
   if (ctmp > cmax) {
      cmax = ctmp;
      imax = i;
   }
}
```

```
cmax = 0.0; imax = -1;
for (i=0; i<1000000; ++i)
   c[i] = a[i] + b[i];
for (i=0; i<1000000; ++i){
   if (c[i] > cmax) {
      cmax = c[i];
      imax = i;
   }
}
```

vectorizable

Loop splitting

- Useful when you want to:
  - remove non-vectorizable components from large computational loops
  - split non-tightly nested loops
- Caveat: does not always work because it increases memory movements

```
for (i=0; i<N; i++){
   a[i] = b[i]*2.0;
   for (j=0; j<M; j++){
      c[i,j] = d[j] + a[i];
   }
}
```

```
for (i=0; i<N; i++){
   a[i] = b[i]*2.0;
}
for (i=0; i<N; i++){
   for (j=0; j<M; j++){
      c[i,j] = d[j] + a[i];
   }
}
```

vectorizable

vectorizable

Loop fusion

- Useful when you want to:
  - get better cache utilization or reuse by minimizing loads and stores
  - increase computational intensity within a loop

```
for (i=0; i<N; ++i){
   for (j=0; j<M; ++j){
      a[i,j] = b[i] + c[j];
   }
}
for (i=0; i<N; ++i){
   for (j=0; j<M; ++j){
      d[i,j] = b[i] - c[j];
   }
}
```

```
for (i=0; i<N; ++i){
   for (j=0; j<M; ++j){
      a[i,j] = b[i] + c[j];
      d[i,j] = b[i] - c[j];
   }
}
```

Inline functions

- A good trick to optimize C++ applications that call small functions
- Eliminate function-call overhead
- Allow the compiler to resolve data dependencies
- How to use:
  1. Define the function as an inline function

```
float add(float a, float b){
  return a+b;
}
```

```
inline float add(float a, float b){
  return a+b;
}
```

  2. Use compiler flags
     Cray: `-hipa[n]. -hipa0` ignores all inlining directives; `-hipa5` most aggressive
     Intel: `-inline`
     GCC: `-finline-functions`
  3. Use compiler directives
     Cray: `#pragma inline_enable`

Make good use of compiler flags and directives

- Modern compilers do many of the optimization techniques
  e.g. loop reordering, unrolling, inlining, etc.
- Can be explicitly specified by the use of directives
- Some common optimization flags to use:
  - `-O0, -O1, -O2, -O3, -Ofast`
  - `-funroll-loops`

- Quick C++ benchmark: http://quick-bench.com/
  An online tool to examine and benchmark effects of different compilers and optimization levels
- Compiler explorer: https://gcc.godbolt.org/
  A website for exploring different compilers and how they generate assembly codes

Aside: How compilers optimize a code?

- To generate vector instructions, compilers:
  1. Identify a construct that performs a series of similar operations (typically a loop)
  2. Perform data dependency analysis
- To convert a series of operations into a vector operation, the operations have to work on a set of data that have been computed upfront

Some good practices:

1. Write codes in a way that hints/makes the compilers to vectorize
2. Avoid items that prevent vectorization by the compiler
   - Loop-carried dependencies
   - Indirect addressing
   - Excessive gathers/scatters/striding within a loop
   - Complex decision processes in a loop
3. Read documentations: https://gcc.gnu.org/onlinedocs/gcc/Optimize-Options.html

```
DO i = 1, N
    a(ia(i)) = b(ib(i)) + c(ic(i))
END DO
```